Catalytic oxidation of VOCs on NaX zeolite: Mixture effect with isopropanol and o-xylene

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ABSTRACT

Catalytic oxidation of isopropanol and o-xylene alone as well as in mixture was investigated over basic NaX zeolite. Experiments were carried out in wet air (11,000 ppm of water) and at a high gas hourly space velocity (GHSV) of 18,000 h^{-1}. Results show an inhibiting effect of the o-xylene on the isopropanol destruction whereas the isopropanol has no effect on the o-xylene destruction. Adsorption experiments as well as molecular modelling seem to demonstrate that this inhibiting effect of o-xylene is due to the adsorption of this aromatic VOCs near the apertures of the NaX supercages limiting the access of isopropanol to the basic active sites of this zeolite. Furthermore, the concentration of o-xylene influences the formation of secondary products (propene, coke) resulting from the isopropanol transformation.

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1. Introduction

Nowadays, the preservation of the quality of air has become a priority as it was shown by the attention and the hopefulness given in the Copenhagen Climate Conference (2009), which unifies 192 countries. Among the emissions of pollutants involved in the air pollution, we can mention the Volatile Organic Compounds (VOCs), which can result from transports, residential/service sector and industry. In the case of industry, emissions are significantly due to the evaporation of solvent during the manufacturing processes, and from a worldwide point of view this tendency is expected to raise in the future [1].

The treatment method to adopt depends on various factors. Catalytic oxidation is usable for low concentrations of VOCs and for a large range of flows. This technique has been widely studied for single compounds and over various catalysts [2–6]. However, only few experiments were carried out on VOCs mixtures treatment [7–13] whereas industrial gas streams often contain mixtures of VOCs of variable composition and concentration. Several studies demonstrated some changes in the reactivity of VOC due to competition phenomenon or reaction between the reactant or/and the products [4,10,11,14,15]. These mixture effects complicate the prediction of the catalyst behaviour.

Over Pt supported on alumina, Dryakhlov and Kiperman [14] described an inhibiting effect of benzene on the destruction of alkanes when the benzene was weakly affected by the presence of alkanes during their oxidation in mixture. This was ascribed to the easier adsorption of the aromatic benzene compared to the dissociative chemisorption of the alkane. Tsou et al. showed that inhibiting effect of the o-xylene on the methyl-isobutyl-ketone should be due to their competition on the active sites and that o-xylene adsorption on metallic sites by the π electrons of the aromatics was certainly favoured in comparison to the ketone [4]. Promoting effect can be observed when chlorinated compounds are oxidized in presence of non-chlorinated hydrocarbons [10] but also when exothermicity is induced at the surface of a catalyst by the oxidation of one or several VOCs. For example, because of the exothermicity, acetone (isopropanol oxidation product) is oxidized at lower temperature in mixture with methylethylketone, toluene and isopropanol [11]. Furthermore, Musialik-Piotrowska and Syczewska [15] found a promoting effect when n-butyl acetate was oxidized in presence of aromatics and alcohol. They suggested that this activation probably resulted from the exothermic character of the complete oxidation reaction, which would locally raise the surface temperature of the catalyst.

Zeolites demonstrated their efficiency as supports or catalysts for the catalytic oxidation of VOCs [16–18]. Recent works showed that basic zeolites such as Faujasite (X or Y type) were good catalysts for VOCs oxidation [18–22]. Faujasite zeolite is composed of SiO_4 and AlO_4^- tetrahedron connected by their oxygen atoms. This crystalline assembly leads to the formation of 8 supercages (α) per unit cell, which create the microporosity of the zeolite. The supercages are assimilated to pseudo sphere 13 Å in diameter with apertures 7.4 Å in diameter. This wide aperture gives access to the micro-

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Table 1
Catalyst characterization.

Catalyst	Formula	Si/Al[a]	Porous volume ($cm^3 g^{-1}$)		Specific surface area ($m^2 g^{-1}$)
			Micro[b]	Meso[c]	
NaX	$Na_{88}Al_{88}Si_{104}O_{384}$	1.2	0.301	0.009	743

[a] Calculated from elementary analysis.
[b] Determined by the *t*-plot method.
[c] Vmeso = Vtotal − VDR (with VDR determined from the Dubinin–Radushkevich equation).

porosity and to the active sites (which are in great part located in the supercages) for a wide range of VOCs such as isopropanol (4.7 Å kinetic diameter) and *o*-xylene (6.6 Å kinetic diameter). The first objective of this work was to study the catalytic oxidation of two VOCs (isopropanol and *o*-xylene) alone and in different mixtures over basic zeolites (NaX Faujasite). Then, on the basis of the observed results we tried to determine (and to explain) the mixture effect on the oxidation of each VOC.

2. Experimental

NaX zeolite (Si/Al = 1.2) was supplied by Axens (Table 1).

Adsorption–desorption isotherms of nitrogen at −196 °C were carried out with a Micromeritics ASAP 2010 apparatus. Micropores volumes were obtained by the *t*-plot method and Dubinin–Radushkevich equation was used to calculate the meso-porosity.

The VOC destruction was carried out in a fixed bed tubular reactor (i.d. = 5 mm, length = 90 cm) at atmospheric pressure and followed as a function of time at constant temperatures, the first point being obtained after 1 min of reaction. The catalyst samples (grain size between 200 μm and 400 μm; catalyst mass = 0.14 g; catalyst bed height = 1.2 cm) were supported on a small plug of glass wool in the vertical reactor. The reactor was inserted into a temperature controlled oven. The temperature was measured by a thermocouple inserted near the catalyst bed. The feed gas (20% O_2 in nitrogen + 1.1% water corresponding to a 33% relative humidity) with the desired mixture concentration of isopropanol and *o*-xylene was introduced in the reactor with a total gas flow rate of 75 mL min^{-1}, which was controlled by a mass flow controller (Brooks, 5850 series). The concentration of VOC was controlled by a CEM Bronkhorst system (liquid mass flow controller followed by an evaporator). The space velocity (GHSV) was kept constant in all the experiments (18,000 h^{-1}, calculated at ambient temperature and pressure).

The analytical system consisted in a gas chromatograph (Varian 3400) equipped with a flame ionization detector for the analysis of the hydrocarbons, and a TCD detector for the analysis of CO_2. The GC was fitted with a 30 m VF-5 ms capillary column, with 0.25 mm of internal diameter and 0.25 μm film thickness.

After reaction, catalyst was recovered and the carbon content deposited on the sample was measured by total burning at 1020 °C, under helium and oxygen, with a CE Instruments NA 2100 Protein analyzer.

Competitive adsorption experiments were also achieved with the same experimental setup, with the same GHSV but at lower temperature (50 °C) and with 210 ppm and 1360 ppm of isopropanol and *o*-xylene, respectively, continuously fed in the reactor. Effect of water vapour addition at a 1.1% concentration was also studied. Breakthroughs of the different VOCs were followed by GC and C/C_0 ratios (outlet/inlet concentrations) were examined to identify eventual competitive desorption phenomena (in that case C/C_0 can transitionally exceed 1 after the initial adsorption step and the subsequent concentration drop). The amounts of VOCs adsorbed or subsequently desorbed were determined by integration with the trapezoid rule of the breakthrough curves.

The modelling results published herewith were generated using the program Cerius^2 version 3.8 developed by Molecular Simulations Inc. The atomic positions for the NaX zeolite were modelled from available X-ray diffraction determination of the dehydrated $[Na_{88}(SiO_2)_{104}(AlO_2)_{88}]$ structure [23]. The substitutional Si, Al disorder in the framework with a Si:Al ratio equal to 1.18 was applied according the Loewenstein rule. The partial atomic charges of the zeolite atoms were taken from previous works [24]. The geometrical parameters for organic molecule modelling have been optimized by *ab initio* calculations at the B3LYP/6-31G** level using the Gaussian 03 software. The SPCE model has been used for modelled water molecules [25]. The interactions between guest molecules and zeolite were modelled by Lennard–Jones (LJ) and Coulombic potentials. For the organic molecules, the LJ potentials are taken from Dreinding forcefield [26] and from the literature for the zeolite oxygen framework [27] and sodium cations [28]. Monte Carlo simulations in the Grand Canonical ensemble (GCMC) followed by energy optimization have been done to model the adsorption of organic molecules and water mixtures in the NaX zeolite. The simulation box consisted in one zeolite unit cell. The behaviour of water, benzene and alkanes in cationic faujasite is well documented and lot of observables and models are available in the literature [28–32]. So, the structure, the sorption sites, the energetics (sorption enthalpy) in cationic zeolites were recalculated for these molecules using the forcefield described above in order to validate the set of parameters and the calculation approximations.

3. Results and discussion

Catalytic oxidation of isopropanol and *o*-xylene was studied over NaX basic zeolites. Firstly, isopropanol (1360 ppm) and *o*-xylene (1360 ppm) destruction was carried out alone over zeolite. Secondly, isopropanol oxidation was performed with the addition of gradual concentration of *o*-xylene (210 ppm and 1360 ppm). Finally, *o*-xylene oxidation was studied, in the same way, with the addition of isopropanol (210 ppm and 1360 ppm).

3.1. Oxidation of single VOCs (isopropanol and o-xylene alone) on NaX

Generally, the destruction of a molecule is correlated to the breaking energy of the weakest C–H bond and to the adsorption enthalpy of the molecule. Thus, the weaker the C–H bond is [33], the stronger the adsorption is [20] and the easier the destruction of the molecule is. In agreement with Papaefthimiou et al. [12] isopropanol should be easier to oxidize than *o*-xylene. Results shown in Table 2 representing the interpolated temperature needed to destroy 50% (T_{50}) of the reactant confirm the results reported in the literature. In fact, the T_{50} of single isopropanol is 70 °C lower that the one obtained for *o*-xylene alone.

However, results show similar CO_2 yield (Fig. 1). These results could be explained by the formation of secondary products and especially from isopropanol.

Indeed and as explained in a previous study [18], the use of basic zeolite as a catalyst to destroy isopropanol leads to acetone and propene, which are more difficult to oxidize than isopropanol.

Table 2
Interpolated temperatures needed to convert 50% (T_{50}) of isopropanol or o-xylene alone and in mixture on NaX zeolite.

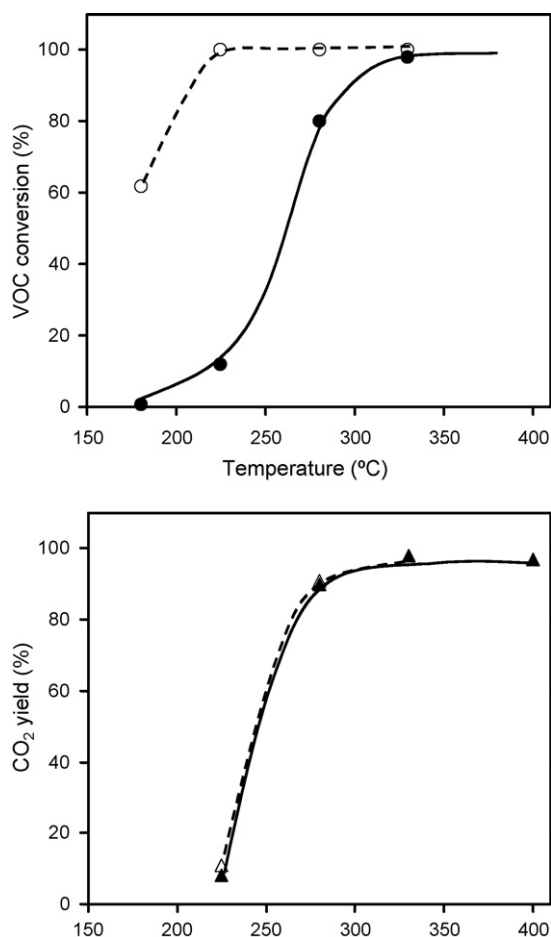|	Isopropanol (1360 ppm)	Isopropanol (1360 ppm) + o-xylene (210 ppm)	Isopropanol (1360 ppm) + o-xylene (1360 ppm)	o-Xylene (1360 ppm) + isopropanol (210 ppm)	o-Xylene (1360 ppm)
T_{50} (isopropanol)	176 °C	224 °C	241 °C	250 °C	–
T_{50} (o-xylene)	–	220 °C	252 °C	252 °C	247 °C

3.2. Effect of isopropanol on o-xylene destruction

Fig. 2 represents the conversion of o-xylene alone (1360 ppm) and in mixture with 210 ppm and 1360 ppm of isopropanol. Results show that o-xylene alone and in mixture is totally destroyed from 330 °C over NaX. It seems that the presence of isopropanol has no effect on the o-xylene conversion and that no significant variation of the T_{50} of is observed when isopropanol is added to 1360 ppm of o-xylene (Table 2). These results seem a priori in agreement with the observations reported by Burgos et al. [11] that showed no effect of isopropanol on the destruction of toluene over Pt/Al$_2$O$_3$ catalysts.
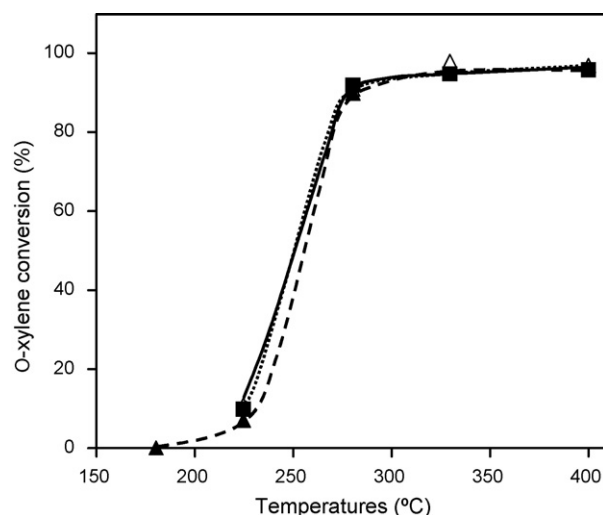
3.3. Effect of o-xylene on isopropanol destruction

Fig. 3 shows that over basic NaX zeolite, very low temperatures are needed to destroy isopropanol. Thus, we can notice the total destruction of this alcohol from 280 °C.

Fig. 3 also shows a decrease of isopropanol destruction when o-xylene is added. Moreover, Table 2 shows that the higher the concentration of o-xylene in the mixture is, the more dif-
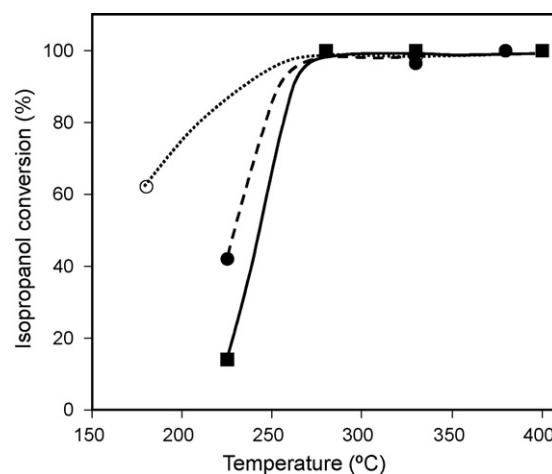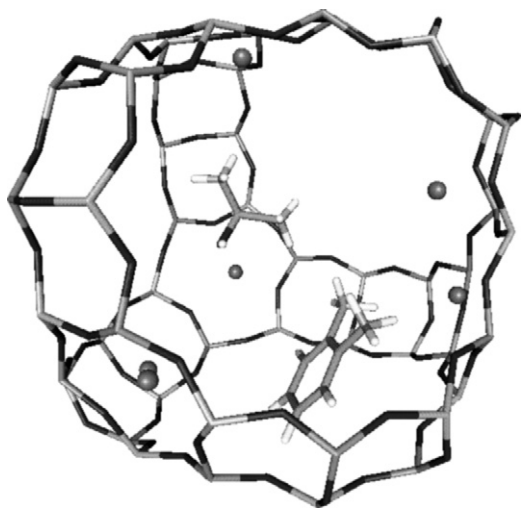

Fig. 2. o-Xylene destruction alone and in mixture as a function of temperatures after 5 h of reaction on NaX with different concentration of isopropanol (1360 ppm o-xylene (△), 1360 o-xylene/210 ppm isopropanol (▲) and 1360 ppm o-xylene/1360 isopropanol (■)).

ficult the destruction of isopropanol is: T_{50} increases from 176 °C (isopropanol alone) to 241 °C (isopropanol/o-xylene mixture 1360 ppm/1360 ppm). It must be underlined that the T_{50} of this latter mixture is close to the one obtained when o-xylene is alone (Table 2). In the case of a competitive adsorption model, these inhibiting effects of o-xylene on the isopropanol destruction could be the result of a competition between isopropanol and o-xylene on the same active sites of the catalyst. In the case of non competitive model (hence on different catalytic sites) conversions could be lowered by a limited access to the active sites because of diffusional limitations, or by the limited intrinsic sites activity (turnover frequency), which would lead to lower conversions

Fig. 1. Temperature influence on the destruction of isopropanol alone (○), o-xylene alone (●) and the CO$_2$ yields obtained (▲ for o-xylene and △ for isopropanol) on NaX after 5 h of reaction.

Fig. 3. Isopropanol destruction alone and in mixture as a function of temperatures after 5 h of reaction on NaX with different concentration of o-xylene (1360 ppm isopropanol (○), 1360 isopropanol/210 ppm o-xylene (●) and 1360 ppm isopropanol/1360 o-xylene (■)).

Fig. 4. Molecular modelling of o-xylene and isopropanol adsorption in a supercage of NaX zeolite in presence of water at 50 °C (only o-xylene and isopropanol molecules are represented, spheres represent Na⁺ cations inside the α supercage).
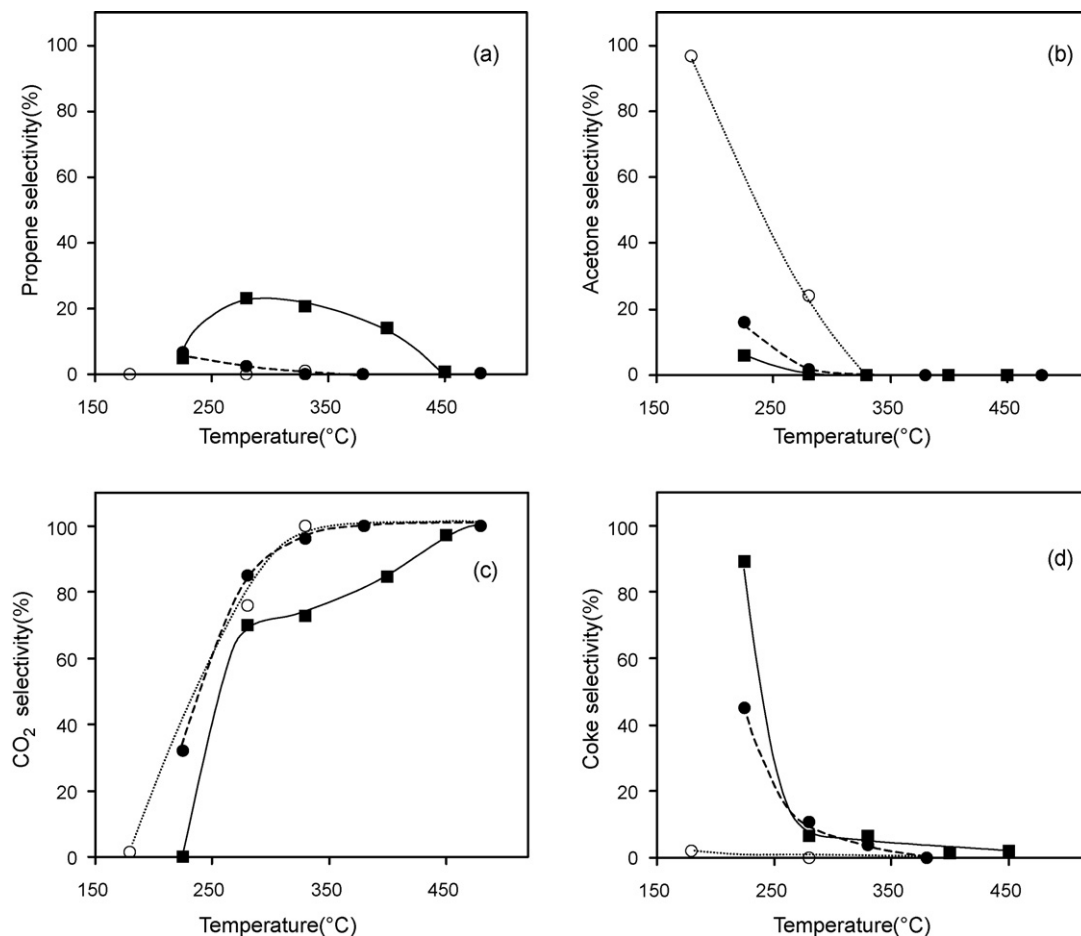
Intrinsic sites activity limitation seems then not to explain our results.

Competitive adsorption between isopropanol and o-xylene in the 210/1360 ppm ratio has then been carried out on NaX catalyst at 50 °C. Results did not show significant competitive desorption of the VOCs in mixture without water addition. The amount of isopropanol adsorbed was 1.07×10^{-3} mol g^{-1} against 5.38×10^{-4} mol g^{-1} for o-xylene.

Then, the same experiment was carried out with water (11,000 ppm). In this case, results showed the total and rapid competitive desorption of isopropanol by water and the partial desorption of o-xylene (1.41×10^{-4} mol g^{-1} remained adsorbed). In presence of water, o-xylene seems therefore to be more strongly adsorbed on the zeolite than isopropanol. Thus, two hypotheses could be done according to the results obtained when water is added to the feed. The first one could be a competitive mechanism that could explain the inhibiting effect of o-xylene observed on the destruction of isopropanol. Another hypothesis could be the adsorption of isopropanol and o-xylene on different sites due to their very different polarity. In that way, the inhibiting effect could result from a steric hindrance, most likely at the pore apertures, due to the presence of o-xylene molecules limiting adsorption and access of isopropanol to the active sites.

3.4. Adsorption modelling

In order to discriminate these hypotheses, adsorption modelling of isopropanol (210 ppm), o-xylene (1360 ppm) and water (1.1%) in mixture was performed on NaX. Firstly, results show

with increasing amounts of VOCs in the feed. According to this latter hypothesis, the increasing amount of o-xylene (with a constant isopropanol concentration) should lead to a decrease of the o-xylene conversion without significant change on the isopropanol conversion. However, T_{50} of o-xylene is only slightly affected whereas T_{50} of isopropanol significantly increases (Table 2).

Fig. 5. Evolution of propene (a), acetone (b), CO$_2$ (c) and coke (d) selectivities obtained from the transformation of 1360 ppm isopropanol (○), 1360 isopropanol/210 ppm o-xylene (●) and 1360 ppm isopropanol/1360 o-xylene (■) as a function of temperatures after 5 h of reaction on NaX.

the better adsorption of water compared to the adsorption of isopropanol and o-xylene. Actually, about 183 water molecules are adsorbed per unit cell (UC), against 6 molecules/UC of isopropanol and 6 molecules/UC of o-xylene. Moreover, the results of modelling (Fig. 4) show that there is an adsorption of isopropanol and water on the cationic site in the supercage when o-xylene is adsorbed near the aperture of the supercage.
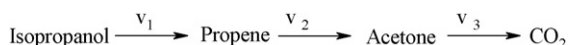
All these results can explain, the total desorption of isopropanol by water, the only partial desorption of o-xylene by water, and the inhibiting effect of o-xylene on isopropanol destruction. Thus, desorption of isopropanol by water could result from the adsorption of isopropanol and H_2O on the same sites and probably the cationic ones. Taking into account the greater polarity of H_2O, its adsorption on these latter sites should be stronger than the one of isopropanol. Indeed, cationic zeolite are well known to be very hydrophilic. However, even if a better adsorption of H_2O than o-xylene on NaX is observed on modelling, experimental results show that o-xylene is not totally desorbed by water. The observations can be explained by the different localisation of o-xylene and water adsorption sites: the adsorption of H_2O occurs on the cations in the supercage whereas o-xylene seems to adsorb near the aperture of the supercage. This leads to a weaker adsorption competition between o-xylene and water than between isopropanol and water. Finally, inhibiting effect of o-xylene over isopropanol conversion seems to be induced by the obstruction of the supercage aperture by o-xylene adsorption, which limits the access of isopropanol to the active sites.

3.5. Conversion of isopropanol into secondary products and into CO_2

During isopropanol oxidation, various compounds are formed: CO_2, propene (resulting from the alcohol dehydration), acetone and coke. Fig. 5 shows the evolution of the selectivities towards these compounds as a function of the reaction temperature and of the composition of the VOCs mixture. When isopropanol is alone, no propene was observed, the amount of acetone decreases with increasing temperature. At low temperature (170 °C) only acetone was detected. On the other hand, this study showed that the mixture has an influence on the formation of secondary products (Fig. 5). Indeed, the presence of o-xylene strongly increases propene formation on NaX basic catalyst, especially above 250 °C and for a high concentration of o-xylene (1360 ppm). Furthermore, coke formation is important at low temperature when the o-xylene concentration is close to 1360 ppm (Fig. 5d). Coke analysis showed that carbon content increases from 0.8 wt% to 2.8 wt% (corresponding to 0.6–2.3% cumulative coke yield) with the addition of 1360 ppm of o-xylene to the isopropanol after 5 h of reaction at 225 °C. Conversely, acetone production decreases when o-xylene is introduced with isopropanol (Fig. 5b).

These results confirm that o-xylene blocks part of the active sites able to oxidize isopropanol (or its by-products) into CO_2 and this especially at low temperature (<350 °C). From these results it is possible to suggest a scheme of isopropanol oxidation (Scheme 1).

Scheme 1 can be commented as follows: isopropanol is rapidly dehydrated into propene (which appears as a primary product of isopropanol transformation in our conditions) even at low temperature (Fig. 5), v_1 is high and the reaction stops at the formation of either acetone or CO_2 (depending on the catalyst and the temperature).

Isopropanol $\xrightarrow{v_1}$ Propene $\xrightarrow{v_2}$ Acetone $\xrightarrow{v_3}$ CO_2

Scheme 1. Oxidation of isopropanol over NaX zeolite.

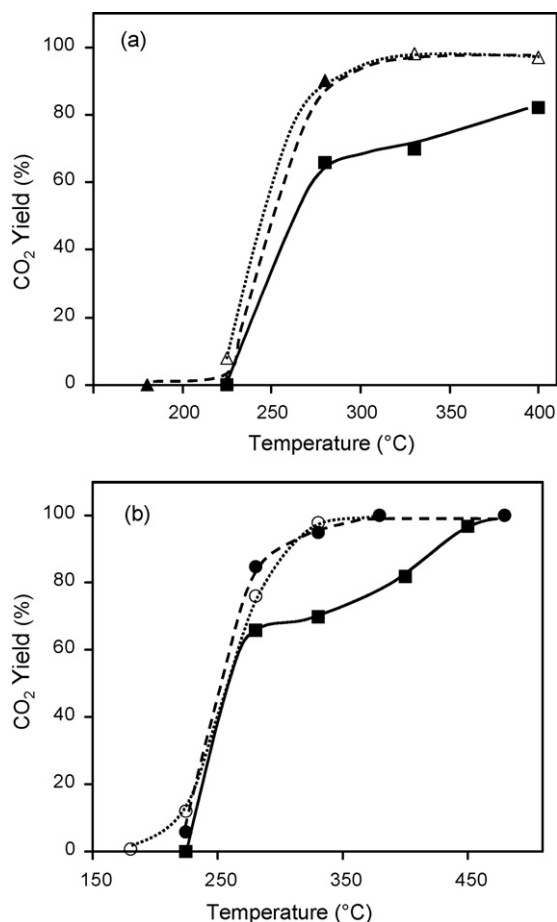**Fig. 6.** Influence of isopropanol addition on the CO_2 yield obtained on NaX (a: o-xylene alone at 1360 ppm (△), o-xylene 1360 ppm/isopropanol 210 ppm (▲) and o-xylene 1360 ppm/isopropanol 1360 ppm (■)) and of o-xylene addition on the CO_2 yield obtained on NaX (b: isopropanol alone at 1360 ppm (○), isopropanol 1360 ppm/o-xylene 210 ppm (●) and isopropanol 1360 ppm/o-xylene 1360 ppm (■)).

The addition of o-xylene leads to two different effects. On one hand, o-xylene location near the aperture of the supercages restricts access of isopropanol to its adsorption site inside the porosity and thus reduces its primary transformation rate (v_1). On the other hand, an inhibiting effect is observed, and propene, which is more difficult to oxidize than o-xylene but exhibits a similar polarity and probably reacts on similar sites, cannot be fully oxidized into acetone. Consequently, v_2 decreases, leading to the observed inversion of the selectivities towards the two reaction intermediates. Moreover, higher residence time could allow the propene to transform into coke. It must be underlined that pyridine adsorption experiments followed by FTIR did not show significant increase in the Brønsted or Lewis acid sites specific bands, which suggests that propene and coke formation were not induced by the creation of acid sites during the pre-treatment of the NaX zeolite at 450 °C.

3.6. CO_2 yield

CO_2 yields presented in Fig. 6 represent the global yields resulting from the oxidation of both isopropanol and o-xylene. No effect of isopropanol on CO_2 conversion was observed on the studied catalysts except in the case of the 1360 ppm isopropanol/1360 ppm o-xylene mixture. The same effect was found when o-xylene was added to isopropanol (Fig. 6b). In the case of the 1360/1360 ppm mixture this effect can be explained by the large formation of

propene, which can be difficult to oxidize because of the presence of *o*-xylene inhibiting the oxidation of propene. The reaction must be then carried out at 450 °C to obtain a total oxidation of the VOCs mixture.

4. Conclusion

This study shows that over basic NaX zeolite no effect of iso-propanol is observed on the destruction of *o*-xylene but that an inhibiting effect of the *o*-xylene presence occurs over isopropanol destruction. According to our results, isopropanol follows a successive oxidation route leading to propene, acetone and finally CO_2. Two phenomena seem to be involved in the observed inhibition process. Firstly, the adsorption of *o*-xylene near the apertures of the supercages of the NaX zeolite seems to limit the access of isopropanol to the sites able to initiate its destruction. Secondly, *o*-xylene competes with propene (resulting from the easy dehydration of isopropanol) on the oxidation sites and consequently increases the selectivity towards propene leading to a lower CO_2 yield and a higher coke formation.

Acknowledgements

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